chain nodes :
    7   8   9   17   18   19   20   21
ring nodes :
    1   2   3   4   5   6   10   11   12   13   14   15
chain bonds :
    2-17   5-7   7-8   7-9   9-11   17-18   17-20   18-19   20-21
ring bonds :
    1-2   1-6   2-3   3-4   4-5   5-6   10-11   10-15   11-12   12-13   13-14   14-15
exact/norm bonds :
    1-2   1-6   2-3   2-17   3-4   4-5   5-6   5-7   7-8   7-9   9-11   10-11   10-15
    11-12   12-13   13-14   14-15   18-19   20-21
exact bonds :
    17-18   17-20
isolated ring systems :
    containing 1 : 10 :

G1:O,N

Match level :
    1:Atom   2:Atom   3:Atom   4:Atom   5:Atom   6:Atom   7:CLASS   8:CLASS   9:CLASS
    10:Atom   11:Atom   12:Atom   13:Atom   14:Atom   15:Atom   17:CLASS   18:CLASS
    19:Atom   20:CLASS   21:Atom

```
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   NEWS  2           "Ask CAS" for self-help around the clock
   NEWS  3   JUL 20  Powerful new interactive analysis and visualization software,
                     STN AnaVist, now available
   NEWS  4   AUG 11  STN AnaVist workshops to be held in North America
   NEWS  5   AUG 30  CA/CAplus -Increased access to 19th century research documents
   NEWS  6   AUG 30  CASREACT - Enhanced with displayable reaction conditions
   NEWS  7   SEP 09  ACD predicted properties enhanced in REGISTRY/ZREGISTRY
   NEWS  8   SEP 22  MATHDI to be removed from STN


   NEWS EXPRESS   JUNE 13 CURRENT WINDOWS VERSION IS V8.0, CURRENT
                  MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
                  AND CURRENT DISCOVER FILE IS DATED 13 JUNE 2005


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   NEWS INTER     General Internet Information
   NEWS LOGIN     Welcome Banner and News Items
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                                                ENTRY        SESSION
FULL ESTIMATED COST                             0.21          0.21

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*                                                                    *
* The CA roles and document type information have been removed from *
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* effective March 20, 2005.  A new display format, IDERL, is now    *
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*                                                                    *
********************************************************************
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for details.

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information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

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=>
Uploading structure

L1      STRUCTURE UPLOADED

=> s l1
SAMPLE SEARCH INITIATED 11:19:04 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -      135 TO ITERATE

100.0% PROCESSED      135 ITERATIONS                         0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:        2003 TO     3397
PROJECTED ANSWERS:              0 TO        0

L2            0 SEA SSS SAM L1

=> s l1 sss full
FULL SEARCH INITIATED 11:20:21 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -     2484 TO ITERATE

100.0% PROCESSED     2484 ITERATIONS                        31 ANSWERS
SEARCH TIME: 00.00.01

L3           31 SEA SSS FUL L1

=> file caplus
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FULL ESTIMATED COST	166.92	167.13

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FILE LAST UPDATED: 30 Sep 2005   (20050930/ED)

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=> s 13
L4              1 L3

=> d 14 bib abs hitstr
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L4   ANSWER 1 OF 1 CAPLUS COPYRIGHT 2005 ACS on STN
Full Text
AN   2004:453187 CAPLUS
DN   141:7141
TI   A preparation of piperazine derivatives, useful as 17β-hydroxysteroid
      dehydrogenase type 3 inhibitors
IN   Paruch, Kamil; Guzi, Timothy J.
PA   Schering Corporation, USA
SO   PCT Int. Appl., 49 pp.
      CODEN: PIXXD2
DT   Patent
LA   English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2004046111	A1	20040603	WO 2003-US36203	20031114

        W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
            CO, CR, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, HR,
            HU, ID, IL, IN, IS, JP, KG, KR, KZ, LC, LK, LR, LT, LU, LV, MA,
            MD, MG, MK, MN, MX, MZ, NI, NO, NZ, PG, PH, PL, PT, RO, RU, SC,
            SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UZ, VC, VN, YU,
            ZA, ZM
        RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ,
            BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE,
            ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK,
            TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

CA 2506290	AA	20040603	CA 2003-2506290	20031114
US 2004127503	A1	20040701	US 2003-713828	20031114
EP 1562901	A1	20050817	EP 2003-783382	20031114

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PRAI US 2002-427263P   P   20021118
     WO 2003-US36203   W   20031114
OS   MARPAT 141:7141
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB   The invention relates to a prepn. of piperazine derivs. of formula I
      [wherein: X is CH or N; Z is O or NH, N-alkyl, or N-aryl, etc.; R1 and R2
      are independently selected from (un)substituted (hetero)aryl,
      (hetero)arylalkyl; R3 is H, OH, alkoxy, aryloxy, etc.; R4 is H,
      (cyclo)alkyl, (hetero)aryl, etc.; R5 is C(O)R6 or SO2R6; R6 is alkyl,

3

(hetero)aryl, (hetero)arylalkyl, (un)substituted amine], useful as
inhibitors of type 3 17β-hydroxysteroid dehydrogenase. The invention
compds. are claimed to be useful for the treatment, prevention,
inhibition, or amelioration of diseases such as prostate cancer, acne, and
androgenic alopecia, etc. The invention compds. exhibited a range of
17β-hydroxysteroid dehydrogenase type 3 binding activity from about
0.005 nM to 10 nM. For instance, piperazine deriv. II was prepd. via
amination of phenyl(trifluoromethylphenyl)methanol by (S)-2-tert-
butylpiperazine (example 7) and subsequent reaction of the obtained
piperazine deriv. III and piperidine deriv. IV (example 15).

IT   696644-18-5P 696644-21-0P 696644-24-3P
      696644-28-7P 696644-32-3P 696644-36-7P
      RL: PAC (Pharmacological activity); PUR (Purification or recovery); SPN
      (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study);
      PREP (Preparation); USES (Uses)
          (prepn. of 17β-hydroxysteroid dehydrogenase type 3 inhibitors for
          the treatment of androgen-dependent diseases)
RN   696644-18-5 CAPLUS
CN   1-Piperidinecarboxylic acid, 4-[[[(2S)-2-(1,1-dimethylethyl)-4-[(S)-
      phenyl[4-(trifluoromethyl)phenyl]methyl]-1-piperazinyl]carbonyl]amino]-,
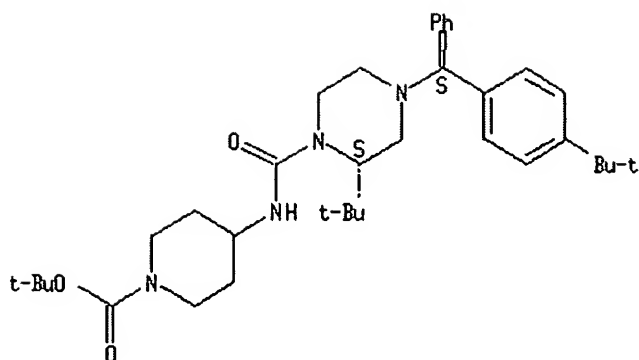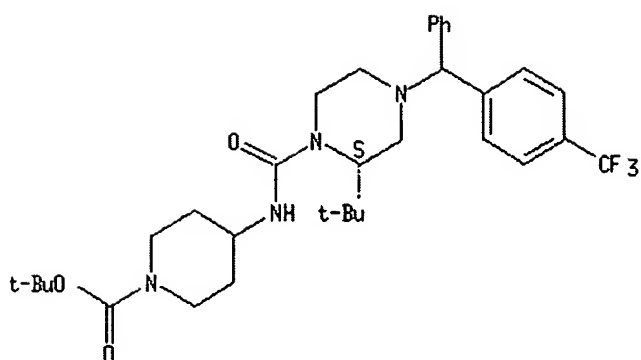   1,1-dimethylethyl ester (9CI)   (CA INDEX NAME)

Absolute stereochemistry.
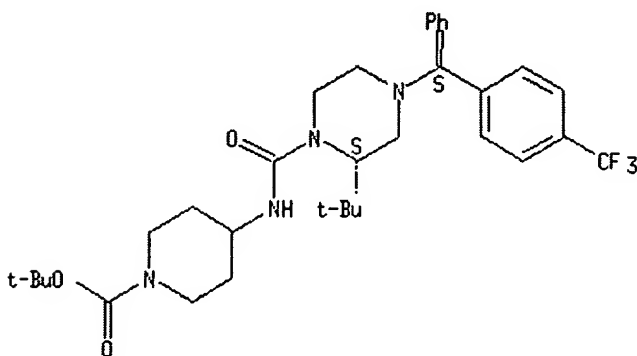
RN   696644-21-0 CAPLUS
CN   1-Piperidinecarboxylic acid, 4-[[[(2S)-2-(1,1-dimethylethyl)-4-[(R)-
      phenyl[4-(trifluoromethyl)phenyl]methyl]-1-piperazinyl]carbonyl]amino]-,
      1,1-dimethylethyl ester (9CI)   (CA INDEX NAME)

Absolute stereochemistry.
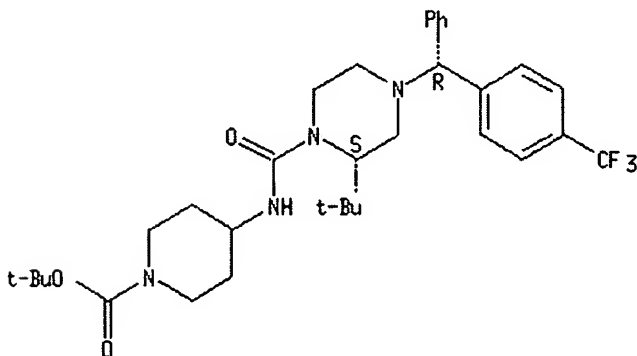
RN   696644-24-3 CAPLUS

CN   1-Piperidinecarboxylic acid, 4-[[[(2S)-2-(1,1-dimethylethyl)-4-[(S)-
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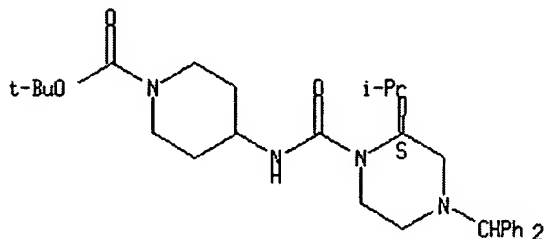   1,1-dimethylethyl ester (9CI)   (CA INDEX NAME)

Absolute stereochemistry.
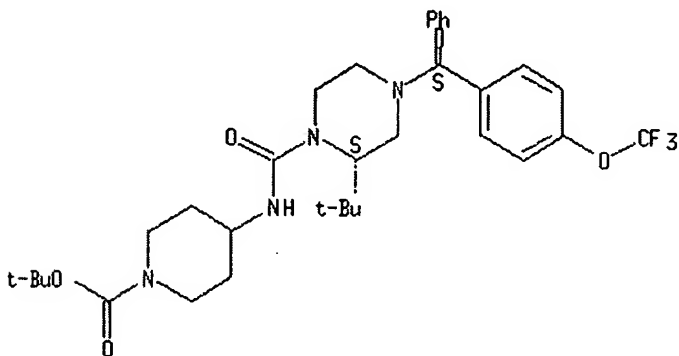
RN   696644-28-7 CAPLUS
CN   1-Piperidinecarboxylic acid, 4-[[[(2S)-2-(1,1-dimethylethyl)-4-[(R)-
     phenyl[4-(trifluoromethoxy)phenyl]methyl]-1-piperazinyl]carbonyl]amino]-,
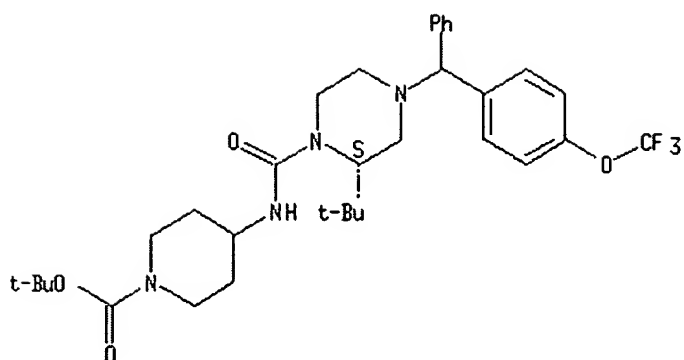   1,1-dimethylethyl ester (9CI)   (CA INDEX NAME)

Absolute stereochemistry.
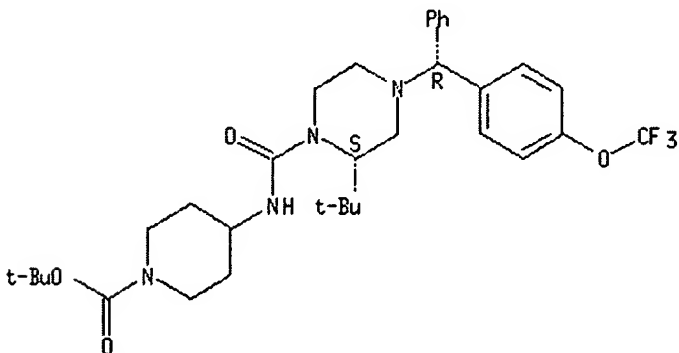
RN   696644-32-3 CAPLUS
CN   1-Piperidinecarboxylic acid, 4-[[[(2S)-2-(1,1-dimethylethyl)-4-[(S)-[4-
     (1,1-dimethylethyl)phenyl]phenylmethyl]-1-piperazinyl]carbonyl]amino]-,
     1,1-dimethylethyl ester (9CI)   (CA INDEX NAME)

Absolute stereochemistry.

RN   696644-36-7 CAPLUS
CN   1-Piperidinecarboxylic acid, 4-[[[(2S)-2-(1,1-dimethylethyl)-4-[(R)-[4-
      (1,1-dimethylethyl)phenyl]phenylmethyl]-1-piperazinyl]carbonyl]amino]-,
      1,1-dimethylethyl ester (9CI)   (CA INDEX NAME)

Absolute stereochemistry.
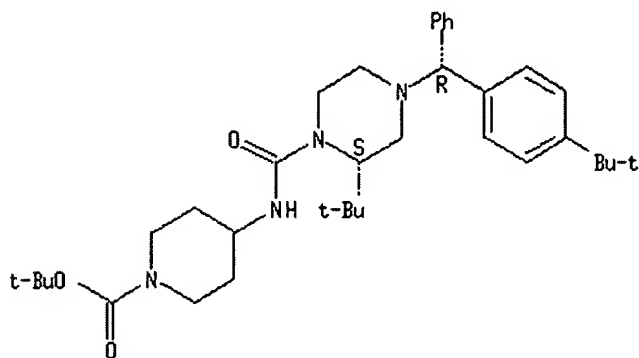
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     696643-88-6P 696643-92-2P 696643-96-6P
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     696644-40-3P 696644-45-8P 696644-50-5P
     696644-54-9P 696644-58-3P 696644-60-7P
     696644-64-1P 696644-66-3P 696644-68-5P
     696644-70-9P 696644-72-1P 696644-78-7P
     696644-82-3P 696644-87-8P 696644-92-5P
     696644-99-2P
     RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
     (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
     (Uses)
        (prepn. of 17β-hydroxysteroid dehydrogenase type 3 inhibitors for
        the treatment of androgen-dependent diseases)
RN   696643-77-3 CAPLUS
CN   1-Piperidinecarboxylic acid, 4-[[[(2S)-2-(1,1-dimethylethyl)-4-[phenyl[4-
      (trifluoromethyl)phenyl]methyl]-1-piperazinyl]carbonyl]amino]-,
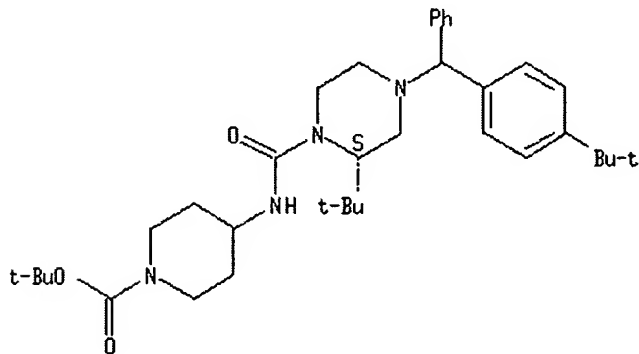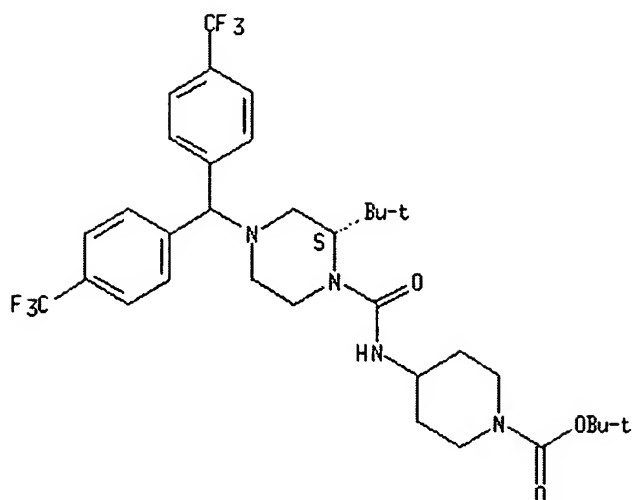   1,1-dimethylethyl ester (9CI)   (CA INDEX NAME)

Absolute stereochemistry.

RN   696643-81-9   CAPLUS
CN   1-Piperidinecarboxylic acid, 4-[[[(2S)-4-(diphenylmethyl)-2-(1-
      methylethyl)-1-piperazinyl]carbonyl]amino]-, 1,1-dimethylethyl ester (9CI)
      (CA INDEX NAME)

Absolute stereochemistry.

RN   696643-85-3   CAPLUS
CN   1-Piperidinecarboxylic acid, 4-[[[(2S)-4-[(4-chlorophenyl)phenylmethyl]-2-
      (1-methylethyl)-1-piperazinyl]carbonyl]amino]-, 1,1-dimethylethyl ester
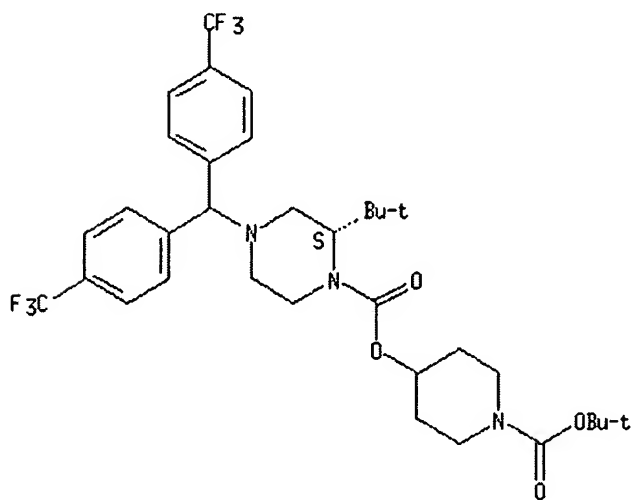   (9CI)   (CA INDEX NAME)

Absolute stereochemistry.
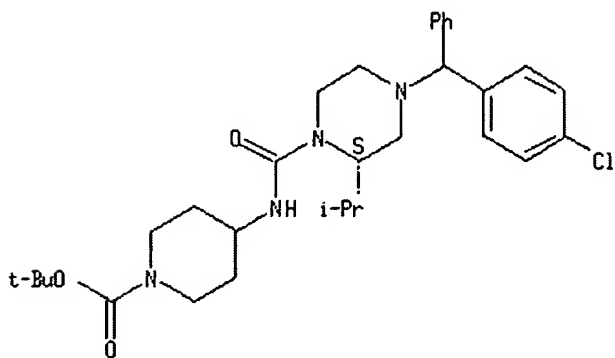
RN   696643-88-6   CAPLUS
CN   1-Piperidinecarboxylic acid, 4-[[[(2S)-2-(1,1-dimethylethyl)-4-[phenyl[4-
      (trifluoromethoxy)phenyl]methyl]-1-piperazinyl]carbonyl]amino]-,
      1,1-dimethylethyl ester (9CI)   (CA INDEX NAME)

Absolute stereochemistry.

RN   696643-92-2   CAPLUS
CN   1-Piperidinecarboxylic acid, 4-[[[(2S)-2-(1,1-dimethylethyl)-4-[[4-(1,1-
      dimethylethyl)phenyl]phenylmethyl]-1-piperazinyl]carbonyl]amino]-,
      1,1-dimethylethyl ester (9CI)   (CA INDEX NAME)
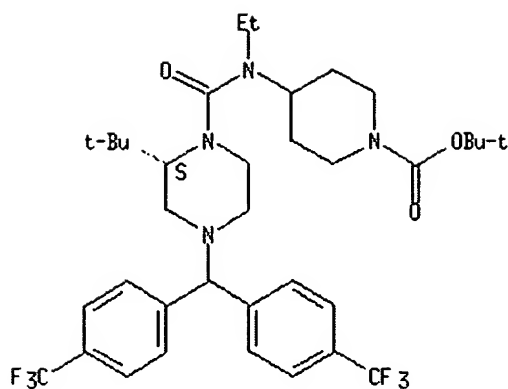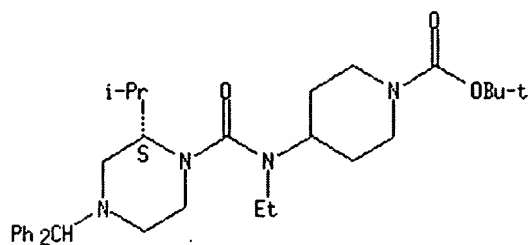
Absolute stereochemistry.

RN   696643-96-6   CAPLUS
CN   1-Piperidinecarboxylic acid, 4-[[[(2S)-4-[bis[4-
      (trifluoromethyl)phenyl]methyl]-2-(1,1-dimethylethyl)-1-
      piperazinyl]carbonyl]amino]-, 1,1-dimethylethyl ester (9CI)   (CA INDEX
      NAME)

Absolute stereochemistry.

RN   696644-00-5 CAPLUS
CN   1-Piperazinecarboxylic acid, 4-[bis[4-(trifluoromethyl)phenyl]methyl]-2-
      (1,1-dimethylethyl)-, 1-[(1,1-dimethylethoxy)carbonyl]-4-piperidinyl
      ester, (2S)- (9CI)   (CA INDEX NAME)

Absolute stereochemistry.

RN   696644-12-9 CAPLUS
CN   1-Piperidinecarboxylic acid, 4-[[[(2S)-4-[bis[4-
      (trifluoromethyl)phenyl]methyl]-2-(1,1-dimethylethyl)-1-
      piperazinyl]carbonyl]ethylamino]-, 1,1-dimethylethyl ester (9CI)   (CA
      INDEX NAME)

Absolute stereochemistry.

RN   696644-15-2 CAPLUS
CN   1-Piperidinecarboxylic acid, 4-[[[(2S)-4-(diphenylmethyl)-2-(1-
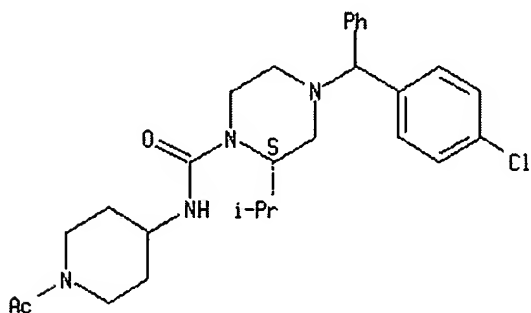   methylethyl)-1-piperazinyl]carbonyl]ethylamino]-, 1,1-dimethylethyl ester
      (9CI)   (CA INDEX NAME)
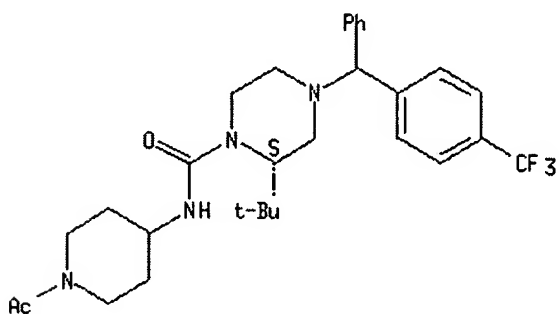
Absolute stereochemistry.

RN   696644-40-3 CAPLUS
CN   1-Piperazinecarboxamide, N-(1-acetyl-4-piperidinyl)-2-(1,1-dimethylethyl)-
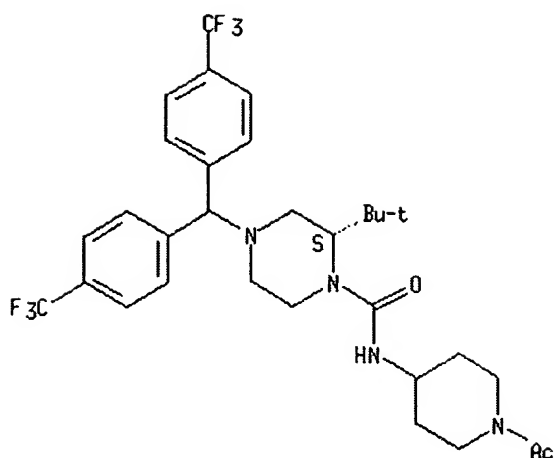   4-[(S)-phenyl[4-(trifluoromethyl)phenyl]methyl]-, (2S)- (9CI)   (CA INDEX
      NAME)

Absolute stereochemistry.
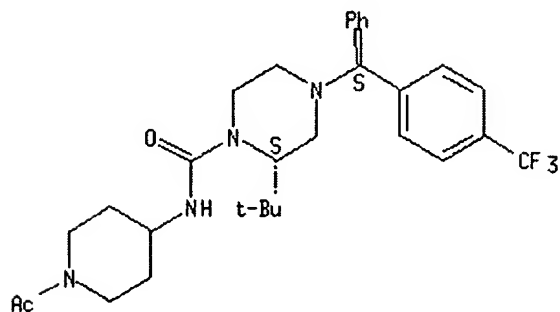
RN   696644-45-8 CAPLUS
CN   1-Piperazinecarboxamide, N-(1-acetyl-4-piperidinyl)-4-(diphenylmethyl)-2-
      (1-methylethyl)-, (2S)- (9CI)   (CA INDEX NAME)

Absolute stereochemistry.

10
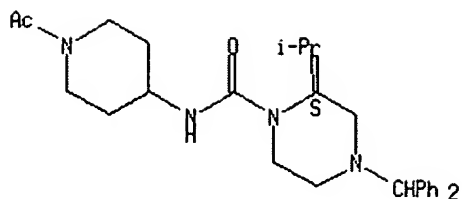
RN   696644-50-5 CAPLUS
CN   1-Piperazinecarboxamide, N-(1-acetyl-4-piperidinyl)-4-[(4-
      chlorophenyl)phenylmethyl]-2-(1-methylethyl)-, (2S)- (9CI)   (CA INDEX
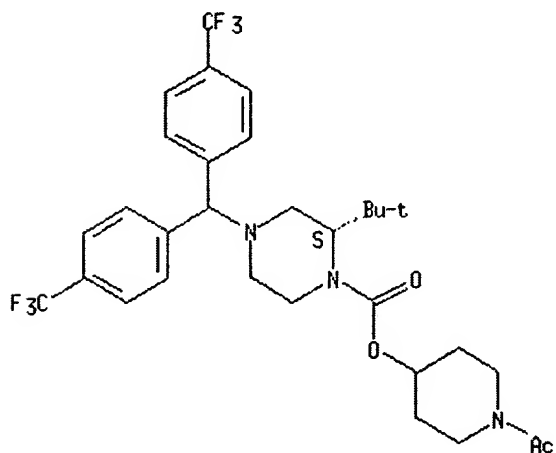   NAME)

Absolute stereochemistry.

RN   696644-54-9 CAPLUS
CN   1-Piperazinecarboxamide, N-(1-acetyl-4-piperidinyl)-2-(1,1-dimethylethyl)-
      4-[phenyl[4-(trifluoromethyl)phenyl]methyl]-, (2S)- (9CI)   (CA INDEX NAME)

Absolute stereochemistry.

RN   696644-58-3 CAPLUS
CN   1-Piperazinecarboxamide, N-(1-acetyl-4-piperidinyl)-4-[bis[4-
      (trifluoromethyl)phenyl]methyl]-2-(1,1-dimethylethyl)-, (2S)- (9CI)   (CA
      INDEX NAME)

Absolute stereochemistry.

RN   696644-60-7 CAPLUS
CN   1-Piperazinecarboxylic acid, 4-[bis[4-(trifluoromethyl)phenyl]methyl]-2-
      (1,1-dimethylethyl)-, 1-acetyl-4-piperidinyl ester, (2S)- (9CI) (CA INDEX
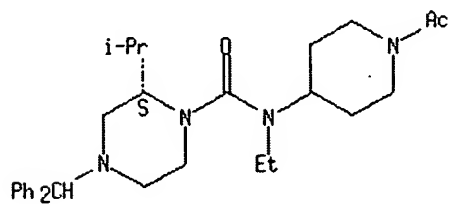   NAME)

Absolute stereochemistry.

RN   696644-64-1 CAPLUS
CN   1-Piperazinecarboxamide, N-(1-acetyl-4-piperidinyl)-4-(diphenylmethyl)-N-
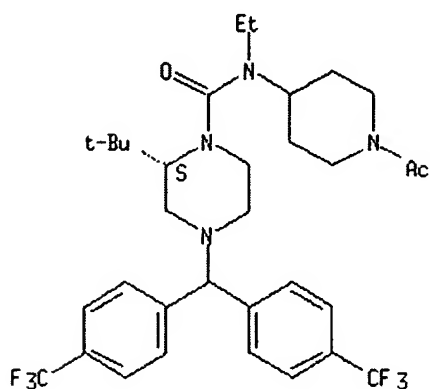   ethyl-2-(1-methylethyl)-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN   696644-66-3 CAPLUS
CN   1-Piperazinecarboxamide, N-(1-acetyl-4-piperidinyl)-4-[bis[4-
      (trifluoromethyl)phenyl]methyl]-2-(1,1-dimethylethyl)-N-ethyl-, (2S)-
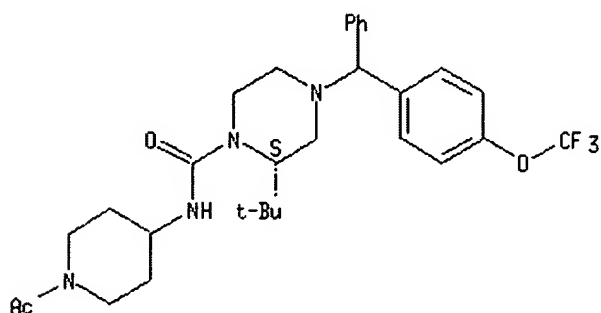
12

(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN   696644-68-5   CAPLUS
CN   1-Piperazinecarboxamide, N-(1-acetyl-4-piperidinyl)-2-(1,1-dimethylethyl)-
      4-[phenyl[4-(trifluoromethoxy)phenyl]methyl]-, (2S)- (9CI)   (CA INDEX
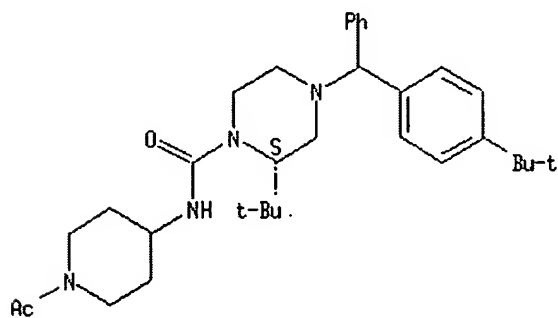   NAME)

Absolute stereochemistry.

RN   696644-70-9   CAPLUS
CN   1-Piperazinecarboxamide, N-(1-acetyl-4-piperidinyl)-2-(1,1-dimethylethyl)-
      4-[[4-(1,1-dimethylethyl)phenyl]phenylmethyl]-, (2S)- (9CI)   (CA INDEX
      NAME)
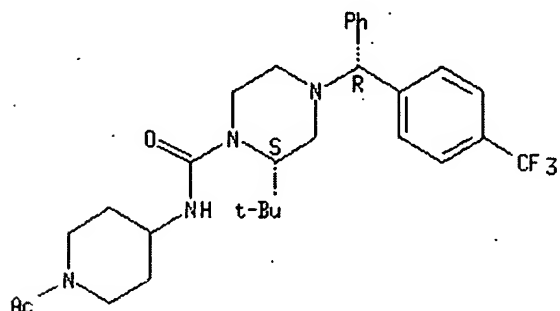
Absolute stereochemistry.

RN   696644-72-1   CAPLUS

CN   1-Piperazinecarboxamide, N-(1-acetyl-4-piperidinyl)-2-(1,1-dimethylethyl)-
     4-[(R)-phenyl[4-(trifluoromethyl)phenyl]methyl]-, (2S)- (9CI)   (CA INDEX
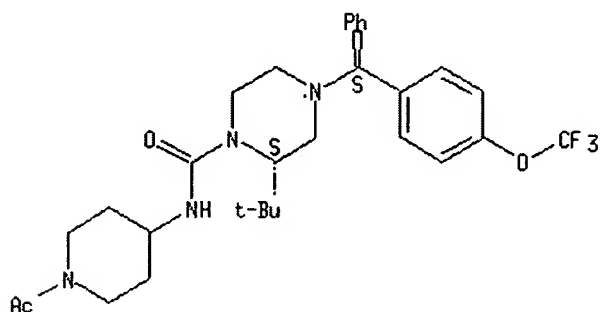   NAME)

Absolute stereochemistry.

RN   696644-78-7   CAPLUS
CN   1-Piperazinecarboxamide, N-(1-acetyl-4-piperidinyl)-2-(1,1-dimethylethyl)-
     4-[(S)-phenyl[4-(trifluoromethoxy)phenyl]methyl]-, (2S)- (9CI)   (CA INDEX
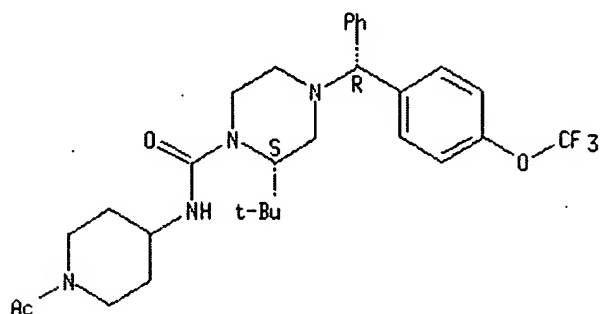   NAME)

Absolute stereochemistry.

RN   696644-82-3   CAPLUS
CN   1-Piperazinecarboxamide, N-(1-acetyl-4-piperidinyl)-2-(1,1-dimethylethyl)-
     4-[(R)-phenyl[4-(trifluoromethoxy)phenyl]methyl]-, (2S)- (9CI)   (CA INDEX
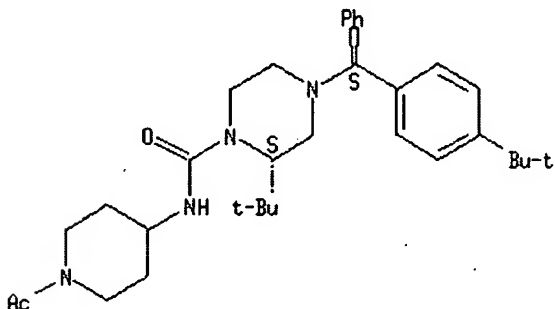   NAME)

Absolute stereochemistry.

RN   696644-87-8   CAPLUS

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CN   1-Piperazinecarboxamide, N-(1-acetyl-4-piperidinyl)-2-(1,1-dimethylethyl)-
      4-[(S)-[4-(1,1-dimethylethyl)phenyl]phenylmethyl]-, (2S)- (9CI) (CA INDEX
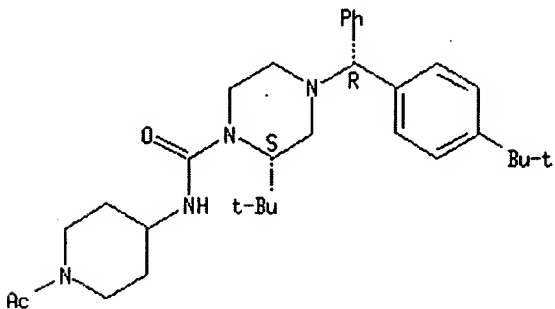   NAME)

Absolute stereochemistry.

RN   696644-92-5 CAPLUS
CN   1-Piperazinecarboxamide, N-(1-acetyl-4-piperidinyl)-2-(1,1-dimethylethyl)-
      4-[(R)-[4-(1,1-dimethylethyl)phenyl]phenylmethyl]-, (2S)- (9CI) (CA INDEX
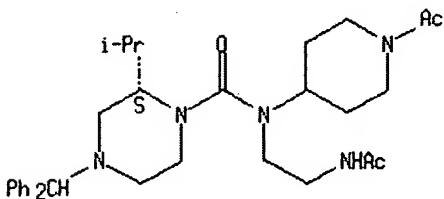   NAME)

Absolute stereochemistry.

RN   696644-99-2 CAPLUS
CN   1-Piperazinecarboxamide, N-[2-(acetylamino)ethyl]-N-(1-acetyl-4-
      piperidinyl)-4-(diphenylmethyl)-2-(1-methylethyl)-, (2S)- (9CI) (CA INDEX
      NAME)

Absolute stereochemistry.

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